Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2021 – 08:11 PM JST

PDB ID	:	7EU9
Title	:	Crystal structure of the selenomethionine(SeMet)-derived Cas12i1 R-loop complex before target DNA cleavage
Authors	:	Zhang, B.; Luo, D.Y.; Li, Y.; OuYang, S.Y.
Deposited on	:	2021-05-16
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

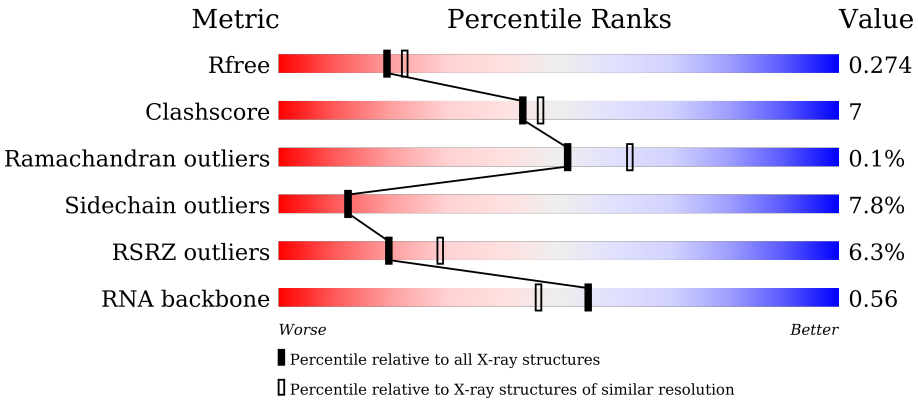
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)
RNA backbone	3102	1006 (2.74-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1101	6% 79% 16%
2	B	43	7% 56% 28% 16%
3	C	40	8% 48% 30% 22%
4	D	40	8% 42% 18% 40%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10849 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cas12i1 D647A mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1078	8720	5549	1508	1623	14	26	0	0	0

- Molecule 2 is a RNA chain called RNA (43-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	43	914	409	158	304	43	0	0	0

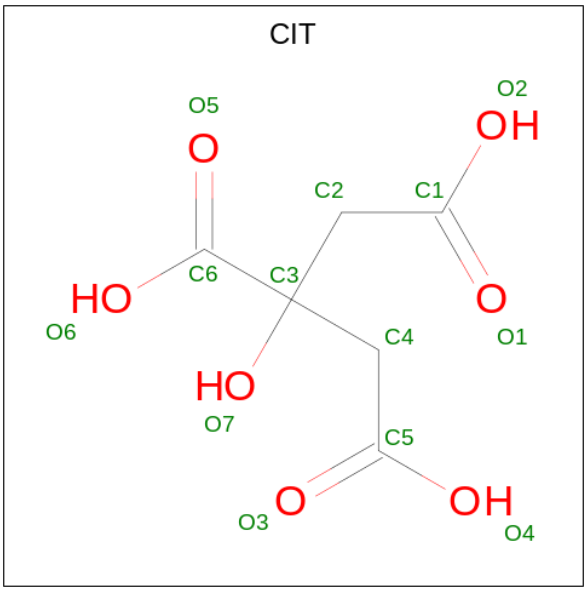
- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	31	629	303	108	187	31	0	0	0

- Molecule 4 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	24	494	235	89	146	24	0	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

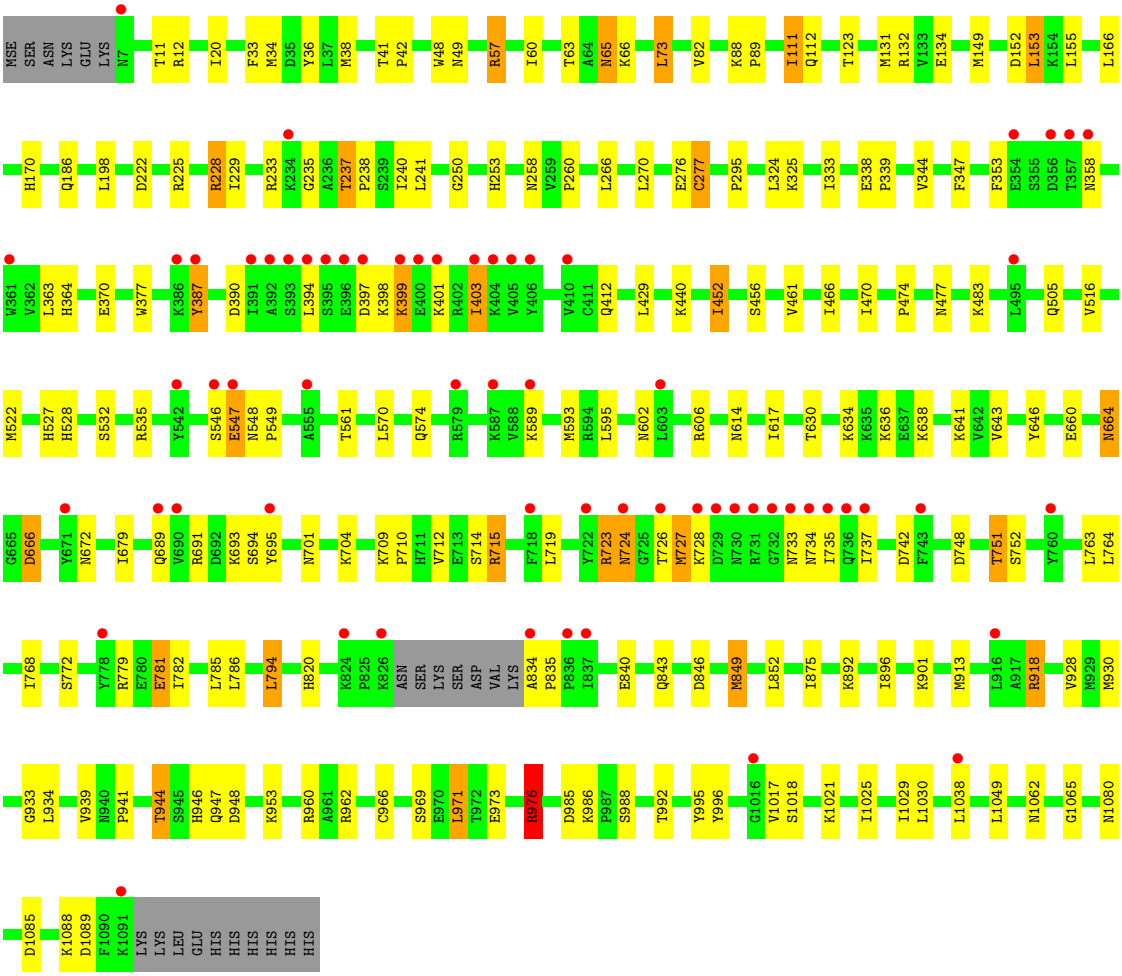
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	69	Total O 69 69	0	0
6	B	3	Total O 3 3	0	0
6	C	3	Total O 3 3	0	0
6	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

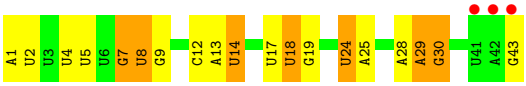
• Molecule 1: Cas12i1 D647A mutant

Chain A:

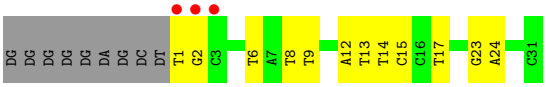


• Molecule 2: RNA (43-MER)

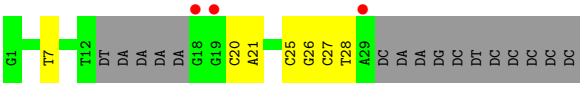
Chain B:



• Molecule 3: DNA (31-MER)



• Molecule 4: DNA (24-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	127.06Å 141.58Å 208.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.63 – 2.35 58.56 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.63-2.35) 99.6 (58.56-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.228 , 0.268 0.237 , 0.274	Depositor DCC
R_{free} test set	3923 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10849	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	0/8872	0.72	0/11896
2	B	0.91	6/1021 (0.6%)	0.84	0/1588
3	C	0.87	4/703 (0.6%)	0.87	0/1081
4	D	0.58	0/552	0.90	0/848
All	All	0.61	10/11148 (0.1%)	0.76	0/15413

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	DC	O3'-P	-7.08	1.52	1.61
2	B	29	A	O3'-P	-6.93	1.52	1.61
3	C	24	DA	O3'-P	-6.22	1.53	1.61
3	C	23	DG	O3'-P	-6.16	1.53	1.61
3	C	12	DA	O3'-P	-6.07	1.53	1.61
2	B	8	U	O3'-P	-5.63	1.54	1.61
2	B	12	C	O3'-P	-5.50	1.54	1.61
2	B	13	A	O3'-P	-5.46	1.54	1.61
2	B	30	G	O3'-P	-5.37	1.54	1.61
2	B	28	A	O3'-P	-5.27	1.54	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	606	ARG	Sidechain
1	A	723	ARG	Sidechain
1	A	918	ARG	Sidechain
1	A	962	ARG	Sidechain
1	A	976	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8720	0	8784	118	0
2	B	914	0	459	10	0
3	C	629	0	353	8	0
4	D	494	0	273	8	0
5	A	13	0	5	3	0
6	A	69	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	4	0	0	0	0
All	All	10849	0	9874	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:GLN:HG2	1:A:593:MSE:HE2	1.52	0.90
1:A:966:CYS:SG	1:A:971:LEU:CD2	2.60	0.90
3:C:6:DT:H5"	3:C:6:DT:H6	1.38	0.89
1:A:483:LYS:NZ	1:A:614:ASN:HD22	1.75	0.83
1:A:225:ARG:O	1:A:229:ILE:HD12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:CYS:SG	1:A:971:LEU:HD22	2.20	0.81
1:A:483:LYS:HZ2	1:A:614:ASN:HD22	1.28	0.79
1:A:849:MSE:CE	1:A:852:LEU:HD23	2.13	0.78
1:A:593:MSE:HE3	1:A:593:MSE:HA	1.68	0.75
1:A:693:LYS:HD3	1:A:695:TYR:OH	1.86	0.74
5:A:1201:CIT:O1	5:A:1201:CIT:O7	2.04	0.74
1:A:849:MSE:HE1	1:A:852:LEU:HD23	1.68	0.74
1:A:240:ILE:HG23	1:A:241:LEU:HD12	1.71	0.72
2:B:18:U:O2'	2:B:19:G:H5"	1.90	0.71
1:A:1025:ILE:O	1:A:1029:ILE:HD12	1.91	0.71
1:A:228:ARG:HH21	1:A:237:THR:HG22	1.53	0.71
3:C:6:DT:H6	3:C:6:DT:C5'	2.05	0.69
1:A:946:HIS:HE1	1:A:996:TYR:OH	1.74	0.69
1:A:941:PRO:O	1:A:944:THR:HB	1.92	0.68
1:A:689:GLN:NE2	1:A:694:SER:HB3	2.08	0.68
3:C:13:DT:H2"	3:C:14:DT:H5'	1.77	0.67
1:A:49:ASN:HB3	1:A:131:MSE:CE	2.26	0.65
1:A:73:LEU:HG	1:A:112:GLN:HB3	1.77	0.65
1:A:834:ALA:N	1:A:835:PRO:CD	2.60	0.65
1:A:399:LYS:H	1:A:399:LYS:HE2	1.63	0.64
1:A:772:SER:HB2	1:A:820:HIS:ND1	2.12	0.64
1:A:470:ILE:HG13	2:B:29:A:H5'	1.79	0.64
4:D:25:DC:H5"	4:D:25:DC:C6	2.32	0.63
1:A:727:MSE:HG3	1:A:737:ILE:HG13	1.81	0.63
1:A:834:ALA:N	1:A:835:PRO:HD2	2.14	0.63
1:A:36:TYR:CE1	1:A:522:MSE:HE1	2.36	0.60
1:A:727:MSE:HG3	1:A:737:ILE:CG1	2.31	0.60
1:A:689:GLN:HE21	1:A:694:SER:HB3	1.67	0.59
4:D:27:DC:H3'	4:D:28:DT:H5"	1.84	0.59
1:A:691:ARG:HH11	2:B:14:U:H3	1.50	0.59
1:A:948:ASP:OD2	1:A:960:ARG:NH2	2.34	0.57
4:D:25:DC:H5"	4:D:25:DC:H6	1.68	0.57
1:A:412:GLN:HA	1:A:412:GLN:OE1	2.05	0.57
1:A:528:HIS:HD2	5:A:1201:CIT:O1	1.88	0.56
1:A:966:CYS:SG	1:A:971:LEU:HD21	2.43	0.56
1:A:547:GLU:OE1	1:A:548:ASN:N	2.36	0.56
1:A:33:PHE:CD2	1:A:516:VAL:HG22	2.41	0.56
1:A:664:ASN:C	1:A:664:ASN:HD22	2.09	0.56
1:A:727:MSE:CG	1:A:737:ILE:HG13	2.36	0.55
1:A:347:PHE:CZ	1:A:353:PHE:HB2	2.40	0.55
4:D:25:DC:C6	4:D:25:DC:C5'	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ARG:NH1	2:B:14:U:H3	2.06	0.54
1:A:849:MSE:HA	1:A:849:MSE:HE3	1.88	0.54
1:A:660:GLU:HB2	1:A:679:ILE:HD11	1.90	0.53
4:D:20:DC:H2'	4:D:21:DA:C8	2.44	0.53
1:A:928:VAL:HG13	1:A:934:LEU:HB3	1.92	0.52
1:A:238:PRO:HG2	1:A:241:LEU:HD13	1.91	0.52
1:A:546:SER:HB3	1:A:602:ASN:HD22	1.75	0.51
1:A:849:MSE:HE2	1:A:852:LEU:HD23	1.91	0.51
1:A:748:ASP:HB2	1:A:751:THR:CG2	2.40	0.51
1:A:715:ARG:NE	1:A:781:GLU:OE2	2.37	0.51
1:A:786:LEU:O	1:A:794:LEU:HB2	2.11	0.51
1:A:170:HIS:HE1	4:D:7:DT:O4	1.93	0.51
1:A:1085:ASP:HB3	1:A:1088:LYS:HD3	1.92	0.51
1:A:295:PRO:HD2	1:A:522:MSE:HE3	1.92	0.51
1:A:477:ASN:HB3	1:A:614:ASN:HD21	1.76	0.50
1:A:724:ASN:OD1	1:A:724:ASN:N	2.31	0.50
1:A:946:HIS:CE1	1:A:996:TYR:OH	2.61	0.50
1:A:973:GLU:CD	1:A:976:ARG:HH22	2.14	0.50
1:A:276:GLU:O	1:A:277:CYS:HB2	2.11	0.50
1:A:38:MSE:HG2	1:A:474:PRO:HG2	1.93	0.50
1:A:701:ASN:O	1:A:752:SER:HB3	2.12	0.50
1:A:764:LEU:O	1:A:768:ILE:HG13	2.11	0.50
1:A:60:ILE:O	1:A:63:THR:HG22	2.11	0.49
1:A:344:VAL:HG11	1:A:452:ILE:HG12	1.94	0.49
1:A:535:ARG:HB2	2:B:7:G:C6	2.47	0.49
1:A:748:ASP:HB2	1:A:751:THR:HG23	1.95	0.49
3:C:6:DT:C5'	3:C:6:DT:C6	2.92	0.49
1:A:344:VAL:HG12	1:A:363:LEU:HD13	1.95	0.49
1:A:483:LYS:NZ	1:A:614:ASN:ND2	2.52	0.49
1:A:390:ASP:HA	1:A:394:LEU:HB2	1.95	0.48
1:A:643:VAL:CG1	1:A:892:LYS:HD3	2.43	0.48
1:A:149:MSE:HE2	1:A:153:LEU:HD13	1.95	0.48
1:A:646:TYR:CE1	1:A:875:ILE:HD11	2.48	0.48
1:A:338:GLU:N	1:A:339:PRO:CD	2.77	0.48
1:A:593:MSE:HA	1:A:593:MSE:CE	2.42	0.48
1:A:149:MSE:HE3	1:A:152:ASP:HB2	1.95	0.48
1:A:709:LYS:N	1:A:710:PRO:CD	2.77	0.47
1:A:896:ILE:O	1:A:918:ARG:HD3	2.15	0.47
1:A:49:ASN:HB3	1:A:131:MSE:HE1	1.95	0.47
3:C:6:DT:H5"	3:C:6:DT:C6	2.30	0.47
1:A:546:SER:CB	1:A:602:ASN:HD22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:U:H2'	2:B:9:G:O4'	2.15	0.46
1:A:20:ILE:HD11	1:A:532:SER:HB3	1.97	0.46
1:A:34:MSE:HE2	1:A:617:ILE:HG22	1.98	0.46
1:A:947:GLN:HB2	1:A:1080:ASN:ND2	2.30	0.46
1:A:250:GLY:HA2	1:A:253:HIS:CD2	2.51	0.46
1:A:250:GLY:HA2	1:A:253:HIS:NE2	2.31	0.46
4:D:26:DG:H2"	4:D:27:DC:H5"	1.98	0.46
1:A:41:THR:HB	1:A:42:PRO:HD3	1.97	0.45
1:A:549:PRO:HA	1:A:602:ASN:HD21	1.81	0.45
1:A:63:THR:HG23	1:A:65:ASN:HD22	1.82	0.45
1:A:364:HIS:ND1	1:A:456:SER:OG	2.44	0.45
2:B:30:G:N2	3:C:17:DT:C2	2.85	0.45
1:A:399:LYS:HE2	1:A:399:LYS:N	2.28	0.45
1:A:333:ILE:CD1	1:A:461:VAL:HG11	2.47	0.44
1:A:12:ARG:HA	1:A:630:THR:O	2.18	0.44
1:A:636:LYS:HB3	1:A:636:LYS:HE3	1.82	0.44
1:A:570:LEU:HG	2:B:18:U:N3	2.32	0.44
1:A:387:TYR:OH	1:A:403:ILE:HD11	2.17	0.44
1:A:727:MSE:HG3	1:A:737:ILE:HD11	1.99	0.44
1:A:1062:ASN:HD21	1:A:1065:GLY:HA2	1.82	0.44
3:C:8:DT:H2'	3:C:9:DT:C6	2.53	0.44
1:A:727:MSE:O	1:A:728:LYS:C	2.56	0.43
1:A:63:THR:HG23	1:A:65:ASN:ND2	2.33	0.43
1:A:483:LYS:HZ3	1:A:614:ASN:HD22	1.64	0.43
3:C:1:DT:H2"	3:C:2:DG:H5'	2.00	0.43
1:A:235:GLY:HA2	4:D:7:DT:O2	2.19	0.43
1:A:892:LYS:HE3	1:A:939:VAL:HG11	2.00	0.43
1:A:527:HIS:ND1	5:A:1201:CIT:H22	2.34	0.43
1:A:782:ILE:HG21	1:A:849:MSE:SE	2.69	0.42
1:A:88:LYS:N	1:A:89:PRO:CD	2.82	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.90	0.42
1:A:733:ASN:OD1	1:A:734:ASN:N	2.52	0.42
1:A:727:MSE:HG3	1:A:737:ILE:CD1	2.49	0.42
1:A:992:THR:HA	1:A:995:TYR:CD2	2.55	0.41
1:A:38:MSE:HE2	1:A:38:MSE:HB3	1.94	0.41
1:A:276:GLU:O	1:A:277:CYS:CB	2.68	0.41
1:A:574:GLN:HG2	1:A:593:MSE:CE	2.38	0.41
1:A:742:ASP:HB3	1:A:763:LEU:HD21	2.01	0.41
1:A:333:ILE:HD11	1:A:461:VAL:HG11	2.02	0.41
1:A:258:ASN:OD1	1:A:260:PRO:HD2	2.21	0.41
1:A:634:LYS:NZ	1:A:934:LEU:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TYR:CD1	1:A:695:TYR:N	2.89	0.41
1:A:111:ILE:HD12	1:A:111:ILE:H	1.85	0.41
1:A:131:MSE:O	1:A:134:GLU:HB2	2.21	0.41
2:B:24:U:O2	2:B:25:A:C8	2.74	0.41
1:A:779:ARG:HD2	1:A:846:ASP:OD2	2.20	0.41
1:A:672:ASN:OD1	1:A:953:LYS:O	2.39	0.40
1:A:933:GLY:O	1:A:934:LEU:HD12	2.21	0.40
1:A:82:VAL:HG21	1:A:466:ILE:HG21	2.02	0.40
2:B:1:A:O5'	2:B:1:A:N3	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1074/1101 (98%)	1025 (95%)	48 (4%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	959/956 (100%)	884 (92%)	75 (8%)	12 12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	48	TRP
1	A	57	ARG
1	A	65	ASN
1	A	66	LYS
1	A	73	LEU
1	A	111	ILE
1	A	123	THR
1	A	153	LEU
1	A	155	LEU
1	A	166	LEU
1	A	186	GLN
1	A	198	LEU
1	A	222	ASP
1	A	233	ARG
1	A	237	THR
1	A	266	LEU
1	A	277	CYS
1	A	324	LEU
1	A	325	LYS
1	A	358	ASN
1	A	370	GLU
1	A	377	TRP
1	A	387	TYR
1	A	397	ASP
1	A	398	LYS
1	A	399	LYS
1	A	401	LYS
1	A	403	ILE
1	A	429	LEU
1	A	440	LYS
1	A	452	ILE
1	A	505	GLN
1	A	547	GLU
1	A	561	THR
1	A	589	LYS
1	A	595	LEU
1	A	638	LYS

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Mol	Chain	Res	Type
1	A	641	LYS
1	A	664	ASN
1	A	666	ASP
1	A	704	LYS
1	A	712	VAL
1	A	714	SER
1	A	715	ARG
1	A	719	LEU
1	A	723	ARG
1	A	724	ASN
1	A	726	THR
1	A	727	MSE
1	A	735	ILE
1	A	751	THR
1	A	781	GLU
1	A	785	LEU
1	A	794	LEU
1	A	840	GLU
1	A	843	GLN
1	A	849	MSE
1	A	901	LYS
1	A	913	MSE
1	A	930	MSE
1	A	944	THR
1	A	969	SER
1	A	971	LEU
1	A	976	ARG
1	A	985	ASP
1	A	986	LYS
1	A	988	SER
1	A	1017	VAL
1	A	1018	SER
1	A	1021	LYS
1	A	1030	LEU
1	A	1038	LEU
1	A	1049	LEU
1	A	1089	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN

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Mol	Chain	Res	Type
1	A	170	HIS
1	A	186	GLN
1	A	358	ASN
1	A	381	ASN
1	A	384	HIS
1	A	505	GLN
1	A	528	HIS
1	A	548	ASN
1	A	602	ASN
1	A	614	ASN
1	A	622	ASN
1	A	649	ASN
1	A	664	ASN
1	A	672	ASN
1	A	689	GLN
1	A	711	HIS
1	A	843	GLN
1	A	946	HIS
1	A	1024	GLN
1	A	1028	ASN
1	A	1062	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	42/43 (97%)	9 (21%)	2 (4%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	4	U
2	B	5	U
2	B	7	G
2	B	14	U
2	B	17	U
2	B	18	U
2	B	24	U
2	B	43	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	4	U
2	B	14	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CIT	A	1201	-	3,12,12	2.16	1 (33%)	3,17,17	4.43	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	1201	-	-	0/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C2-C3	-3.48	1.50	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1201	CIT	C3-C2-C1	-7.40	103.14	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	CIT	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1052/1101 (95%)	0.52	63 (5%) 21 32	31, 54, 100, 166	0
2	B	43/43 (100%)	0.37	3 (6%) 16 24	38, 50, 81, 140	0
3	C	31/40 (77%)	0.43	3 (9%) 7 12	39, 50, 175, 187	0
4	D	24/40 (60%)	0.74	3 (12%) 3 6	40, 73, 151, 173	0
All	All	1150/1224 (93%)	0.51	72 (6%) 20 29	31, 54, 104, 187	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	732	GLY	9.4
1	A	734	ASN	8.6
1	A	733	ASN	8.5
1	A	730	ASN	7.8
1	A	729	ASP	7.5
1	A	403	ILE	7.5
1	A	397	ASP	7.4
1	A	399	LYS	7.4
1	A	737	ILE	7.1
1	A	826	LYS	6.2
1	A	731	ARG	5.8
1	A	394	LEU	5.5
1	A	735	ILE	5.2
4	D	18	DG	5.1
1	A	736	GLN	5.0
1	A	393	SER	5.0
1	A	395	SER	5.0
1	A	356	ASP	4.9
2	B	43	G	4.4
1	A	724	ASN	3.9
3	C	2	DG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	410	VAL	3.8
3	C	1	DT	3.8
1	A	555	ALA	3.7
3	C	3	DC	3.5
1	A	587	LYS	3.4
1	A	603	LEU	3.4
1	A	406	TYR	3.3
1	A	1091	LYS	3.2
1	A	354	GLU	3.1
1	A	404	LYS	3.0
1	A	392	ALA	2.9
1	A	546	SER	2.9
4	D	19	DG	2.9
1	A	396	GLU	2.9
1	A	358	ASN	2.8
1	A	728	LYS	2.8
1	A	834	ALA	2.8
1	A	718	PHE	2.7
1	A	391	ILE	2.7
1	A	386	LYS	2.7
1	A	357	THR	2.6
1	A	760	TYR	2.6
4	D	29	DA	2.6
1	A	778	TYR	2.6
1	A	401	LYS	2.5
1	A	7	ASN	2.4
1	A	1038	LEU	2.4
1	A	689	GLN	2.4
1	A	836	PRO	2.4
1	A	387	TYR	2.4
1	A	824	LYS	2.4
1	A	1016	GLY	2.3
1	A	547	GLU	2.3
1	A	695	TYR	2.3
1	A	361	TRP	2.3
1	A	726	THR	2.2
1	A	400	GLU	2.2
2	B	41	U	2.2
1	A	916	LEU	2.2
1	A	589	LYS	2.2
1	A	690	VAL	2.2
2	B	42	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	495	LEU	2.2
1	A	743	PHE	2.1
1	A	405	VAL	2.1
1	A	837	ILE	2.1
1	A	542	TYR	2.1
1	A	234	LYS	2.0
1	A	579	ARG	2.0
1	A	671	TYR	2.0
1	A	722	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	A	1201	13/13	0.86	0.15	42,65,76,78	0

6.5 Other polymers (i)

There are no such residues in this entry.